1. Record Nr. UNINA9910141639403321

Autore	Albright Thomas A
Titolo	Orbital interactions in chemistry / / by Thomas A. Albright, Jeremy K. Burdett, Myung-Hwan Whangbo
Pubbl/distr/stampa	Hoboken, N.J., : John Wiley & Sons, c2013
ISBN	9781118558256 1118558251 9781118558409 1118558405 9781118558218 1118558219
Edizione	[2nd ed.]
Descrizione fisica	1 online resource (835 p.)
Classificazione	SCI013050
Altri autori (Persone)	BurdettJeremy K WhangboMyung-Hwan
Disciplina	541/.28
Soggetti	Molecular orbitals
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes index.
Nota di contenuto	Orbital Interactions In Chemistry; Contents; Preface; About the Authors; Chapter 1: Atomic and Molecular Orbitals; 1.1 Introduction; 1.2 Atomic Orbitals; 1.3 Molecular Orbitals; Problems; References; Chapter 2: Concepts of Bonding and Orbital Interaction; 2.1 Orbital Interaction Energy; 2.1.1 Degenerate Interaction; 2.1.2 Nondegenerate Interaction; 2.2 Molecular Orbital Coefficients; 2.2.1 Degenerate Interaction; 2.2.2 Nondegenerate Interaction; 2.3 The Two-Orbital Problem-Summary; 2.4 Electron Density Distribution; Problems; References; Chapter 3: Perturbational Molecular Orbital Theory 3.1 Introduction3.2 Intermolecular Perturbation; 3.3 Linear H3, HF, and the Three-Orbital Problem; 3.4 Degenerate Perturbation; Problems; References; Chapter 4: Symmetry; 4.1 Introduction; 4.2 Symmetry of Molecules; 4.3 Representations of Groups; 4.4 Symmetry Properties of Orbitals; 4.5 Symmetry-Adapted Wavefunctions; 4.6 Direct Products; 4.7 Symmetry Properties, Integrals, and the Noncrossing Rule; 4.8 Principles of Orbital Construction Using Symmetry Principles; 4.9 Symmetry Properties of Molecular Vibrations; Problems; References

Chapter 5: Molecular Orbital Construction from Fragment Orbitals5.1 Introduction; 5.2 Triangular H3; 5.3 Rectangular and Square Planar H4; 5.4 Tetrahedral H4; 5.5 Linear H4; 5.6 Pentagonal H5 and Hexagonal H6; 5.7 Orbitals of Cyclic Systems; Problems; References; Chapter 6: Molecular Orbitals of Diatomic Molecules and Electronegativity Perturbation; 6.1 Introduction; 6.2 Orbital Hybridization; 6.3 Molecular Orbitals of Diatomic Molecules; 6.4 Electronegativity Perturbation; 6.5 Photoelectron Spectroscopy and Through-Bond Conjugation; Problems; References
Chapter 7: Molecular Orbitals and Geometrical Perturbation7.1 Molecular Orbitals of AH2; 7.2 Geometrical Perturbation; 7.3 Walsh Diagrams; 7.4 Jahn-Teller Distortions; 7.4.1 First-Order Jahn-Teller Distortion; 7.4.2 Second-Order Jahn-Teller Distortion; 7.4.3 Three-Center Bonding; 7.5 Bond Orbitals and Photoelectron Spectra Of AH2 Molecules; Problems; References; Chapter 8: State Wavefunctions and State Energies; 8.1 Introduction; 8.2 The Molecular Hamiltonian and State Wavefunctions; 8.3 Fock Operator; 8.4 State Energy; 8.5 Excitation Energy; 8.6 Ionization Potential and Electron Affinity
8.7 Electron Density Distribution and Magnitudes of Coulomb and Exchange Repulsions8.8 Low versus High Spin States; 8.9 Electron-Electron Repulsion and Charged Species; 8.10 Configuration Interaction; 8.11 Toward More Quantitative Treatments; 8.12 The Density Functional Method; Problems; References; Chapter 9: Molecular Orbitals of Small Building Blocks; 9.1 Introduction; 9.2 The AH System; 9.3 Shapes of AH3 Systems; 9.4 -Bonding Effects of Ligands; 9.5 The AH4 System; 9.6 The AHn Series-Some Generalizations; Problems; References; Chapter 10: Molecules with Two Heavy Atoms; 10.1 Introduction
10.2 A2H6 Systems

Sommario/riassunto

Explains the underlying structure that unites all disciplines in chemistry Now in its second edition, this book explores organic, organometallic, inorganic, solid state, and materials chemistry, demonstrating how common molecular orbital situations arise throughout the whole chemical spectrum. The authors explore the relationships that enable readers to grasp the theory that underlies and connects traditional fields of study within chemistry, thereby providing a conceptual framework with which to think about chemical structure and reactivity problems. Orbital Interactions